Butyl nitrate 928-45-0 | DTXSID70239143

		1	
Model Performance			

Model

Weighted KNN model

Data

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.91	1.08	0.91	1.08	0.92	1.00	

Model Results

Predicted value: 10.7 mmHg

Global applicability domain: Inside

Local applicability domain index: 8.04e-01

Confidence level: 7.81e-01

Nearest Neighbors from the Training Set

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6-Undecanone Measured: 8.30 Predicted: 6.95e-02

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Butanedioyl dichloride Measured: 8.30 Predicted: 1.92e-01

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Propyl carbamate Measured: 23.5 Predicted: 9.85e-02

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Clopyralid Measured: 34.1 Predicted: 3.04e-04

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Fosthietan Measured: 5.13 Predicted: 2.14e-05